Quasiperiodic Nanoscale Faceting of High-Index Si Surfaces

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Scanning tunneling microscopy reveals that Si(112) reconstructs into quasiperiodic, nanometer-scale facets. Each sawtoothlike facet consists of a single unit cell wide reconstructed (111) terrace (7×7 or 5×5) opposed by a 60 to 110 Å wide (337) terrace. Nanofacets with a similar structure are also observed on Si(335), indicating that they are a general phenomenon for some range of vicinality towards $[\bar{1}\bar{1}2]$. The dimensions of these nanofacets suggest that Si(112) and Si(335) would be interesting substrates for the growth of corrugated superlattices.

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There is considerable interest in vicinal semiconductor surfaces as potential substrates for electronic device fabrication [1]. The uniformly spaced distribution of steps on a bulk-terminated vicinal surface is expected to promote step-flow growth during heteroepitaxy, and to provide a natural template for the growth of spatially confined structures. Unfortunately, vicinal semiconductor surfaces usually have terrace length distributions far from ideal. Such surfaces typically consist of large low-index terraces separated by multilayer-height steps or step bunches [2–4], as opposed to periodic short terraces separated by single-layer-height steps (expected in the bulk-terminated case).

Two high-index surfaces of Si, the (113) and (112), are thought to be relatively stable [4–9], and have therefore been used as substrates for the growth of high-quality III-V semiconductor epilayers [10,11] and possible quantum well wire arrays [12]. It has been shown via scanning tunneling microscopy (STM) studies that a complex reconstruction stabilizes the (113) surface orientation [7]. STM studies of the (112) surface, however, have yet to result in a model for the structure of this crystal face. [A model of the bulk-terminated (112) surface is shown in Fig. 1.] While one STM study of Si(112) observed a large number of (111) terraces along with a variety of other unidentified structures [13], a second study reported a (1×2) reconstruction with a longer period, pseudo-ordered domain structure [9]. In this Letter we report the results of our atomic-resolution STM study of Si(112). We find that clean, well-ordered surfaces exhibit a novel quasiperiodic reconstruction consisting of sawtoothlike nanofacets composed of short (337)- and (111)-oriented terraces. Furthermore, we observe a nearly identical reconstruction on Si(335), suggesting that this nanoscale faceting is a general phenomenon for some range of vicinality towards [112].

The experiments were performed in ultrahigh vacuum (UHV) on Si wafers oriented to within 0.5° of (112) (as verified by x-ray diffraction) or (335). The samples were precleaned in a boiling 1:3 solution of H_2O_2 and H_2SO_4, rinsed in distilled water, and then blown dry with nitrogen. Each sample was then mounted on a button heater in UHV, outgased at 600 °C for 1 h, flashed to ≈1150 °C for 60 s with the pressure $\leq 2 \times 10^{-9}$ Torr, and then cooled at rates from 15 to <0.5 °C/s. Atomic-resolution STM images of both the empty and filled electronic states were acquired at room temperature with a constant current of 0.1–0.3 nA and bias voltages between 1.0 and 2.5 V. All images presented here are three-dimensionally rendered topographs of the filled states.

Images of slowly cooled Si(112) surfaces are presented in Fig. 2, revealing that Si(112) has a much more complicated structure than the bulk-terminated case. As shown in the large-scale image [Fig. 2(a)], two distinct structural regions are observed, labeled "I" and "II," neither of which contain (112)-oriented terraces. Closer inspection of type-I regions [Fig. 2(b)] shows a sawtoothlike structure with

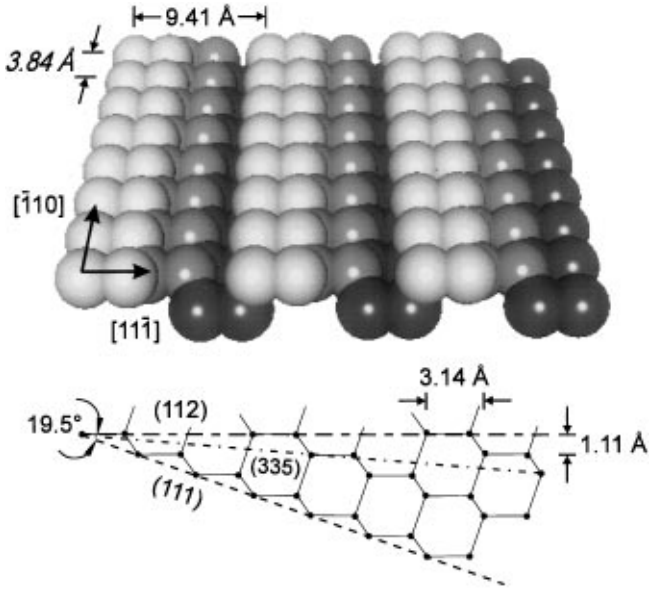

FIG. 1. A model of the bulk-terminated Si(112) surface. The bulk-terminated surface, which can be thought of as Si(111) tilted 19.5° towards [112], would consist of 8.87 Å wide (111) terraces separated by 3.14 Å high (001)-oriented steps. In the (112) plane the unit cell is 3.84 Å × 9.41 Å. The – – · – – line indicates the (335) plane.

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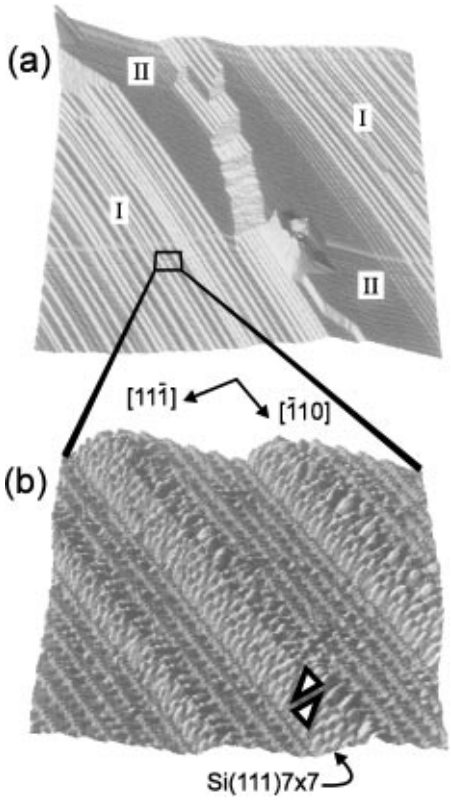

FIG. 2. Rendered STM topographs of Si(112). (a) 5000 Å × 5000 Å image (340 Å height range) showing regions of quasiperiodic nanofacets (I) which are believed to be the equilibrium surface structure, and two large terraces (II) pinned by trace contaminants. (b) 320 Å × 270 Å image (12 Å height range) of the nanofacets (filled states) showing a sawtoothlike structure. One 7 × 7 unit cell on the (111) side of a sawtooth is highlighted. Note that this image is of a different sample than (a); the box is shown to indicate relative scale.

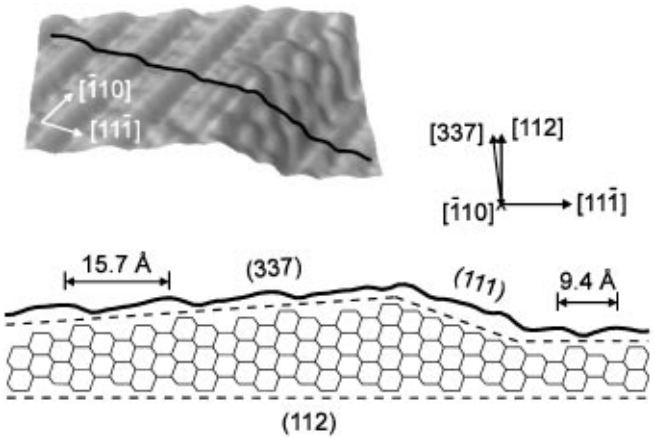

FIG. 3. Quantitative analysis of the nanofacet structure on Si(112). An image approximately 100 Å × 40 Å (≈10 Å height range) is shown along with a profile of the topography. The profile is also displayed over a cross section of the Si crystal structure, showing that the sawtooth is composed of short (111) and (337) facets.

an approximate period of 130 Å and depth of 8 Å. The longer sides of the sawtooths have a narrow width distribution in the [11$\bar{1}$] direction, ranging from 60 to 110 Å, and are dominated by prominent rows of atomic-scale features running along [110]. The shorter sides of the sawtooths are one unit cell wide 7 × 7 or 5 × 5 reconstructed Si(111) planes. Type-II regions consist of large terraces (up to ~1000 Å wide) which are pinned by an aggregation of contaminants. These pinned terraces have a novel structure with a net orientation a few degrees away from the underlying (112), which will be discussed in detail in a separate publication [14]. We believe that the quasiperiodic nanofacets (type-I regions) are the equilibrium structure of the clean Si(112) surface [15].

The well-resolved 7 × 7 and 5 × 5 reconstructions observed on the (111) sides of the nanofacets provide an absolute calibration of the length scales in the STM images, independent of thermal drift, piezo calibration, etc. This enables the structure of the nanofacets to be determined, as illustrated in Fig. 3. An image of a nanofacet (cropped from a much larger topograph) is rendered along with a profile of its topography. The profile was taken from the raw data following subtraction of a simple planar background. Note that profiles taken from a variety of unprocessed images acquired with different tunneling tips and substrates are all quite similar. As shown in Fig. 3, a profile can be *absolutely* scaled simply by adjusting the height scale so that the segment of the profile spanning the (111) facet has the correct aspect ratio. Since the width vs height of a (111) 7 × 7 unit cell with respect to the (112) basal plane is determined by the Si crystal structure, *this transformation is unique.* The analysis shows that the longer side of the nanoscale facet is 4.0° steeper than (112) and has a unit cell that is 15.7 Å wide along [111], corresponding to the (337) plane.

The accuracy of this analysis is indicated by the excellent fit of the adjusted profile to the correctly scaled side view of the underlying (337)-(111) crystal structure. Note that the bulk-terminated views shown are only intended to illustrate the expected periodicity; possible atomic-scale models of the reconstructed (337) surface will be discussed elsewhere [14]. The profile shown in Fig. 3 has an additional feature that confirms the accuracy of the analysis: a one unit cell wide region of a horizontal (112) "plane" with the expected width of 9.4 Å. [Such regions are very infrequently observed adjacent to the (111) facets.]

The narrow width distribution of the nanofacets can be understood by examining the crystal structure as projected onto the (112) surface. In this projection the Si crystal lattice is composed of units $a = 3.14$ Å wide by $c = 1.11$ Å high (see Fig. 1). Using these units, each (111) 7 × 7 unit cell is $7a$ wide and $7c$ high, while each (337) unit cell is $5a$ (15.7 Å) wide and c high. Therefore, in order to maintain the (112) sample orientation, a "perfect" nanofacet must be composed of seven units of (337) for each unit of 7 × 7 [or similarly, five units of (337) for each unit of 5 × 5]. Since the (111) plane has its lowest energy when 7 × 7 reconstructed, an integral number of

7×7 unit cells are expected on the (111) sides of the nanofacets. In fact, all the (111) sides of the nanofacets we observe are only a *single* 7×7 (or 5×5) unit cell wide [16]. In combination with the above requirements of the crystal structure, this gives the nanofacets their characteristic length scale.

Although the (111) sides of the nanofacets are uniformly $7a = 22$ Å wide, the (337) sides are not uniformly $7 \times 5a = 110$ Å wide for a variety of reasons. For example, the (112) orientation is not perfectly maintained within each nanofacet: The (337) sides are sometimes one or two unit cells shorter or longer than ideal. In addition, a different structure that is $7a$ wide by $2c$ high [corresponding to a single unit cell of (225)] is often observed on the (337)-like sides, usually occurring on the longer terraces. This structure shortens by $3a$ the length required to compensate for the height of the 7×7 unit cell, probably reducing the strain associated with the nanofacet. In addition to the occasional (225) unit cell, a few other structures are infrequently observed on the (337) terraces as well, including single unit cells of (112) and (559). These phenomena give rise to the observed width distribution of the (337)-(111) nanofacets.

In order to investigate whether the novel nanometer-scale faceting observed on Si(112) is unique to that vicinal surface, we have also examined Si(335). As indicated in Fig. 1, the (335) plane is tilted only 14.4° from the (111) plane, as compared to (112) which is tilted 19.5° towards [112]. Note that surfaces tilted up to 7.7° consist of large (111) 7×7 terraces separated by single- or triple-layer-height steps [3]. Surprisingly, we find that the (335) surface reconstructs into nanoscale facets very similar to those observed on Si(112). In Fig. 4(a) a large-scale image of a slowly cooled Si(335) surface is displayed, identical in scale to the image of Si(112) shown in Fig. 2(a). Since the slight miscut of the Si(335) wafer results in step bunches that tend to run along the [111] direction, they do not significantly affect the width of the nanofacets [17]. From the atomic-resolution view of the (335) surface shown in Fig. 4(b), it is clear that this surface has a (337)-(111) structure similar to that on Si(112), but with a shorter period (≈60 Å) and shallower depth (≈6 Å).

The two most apparent differences between nanofacets on the (335) vs (112) surfaces are the much shorter (337)-like sides and the larger regions of disorder at the top of the nanofacets. Both of these differences can be accounted for by considering the different coincidences of these surfaces with respect to the (337) and (111) planes, as illustrated in Fig. 5. While an ideal nanofacet composed of seven unit cells of (337) and one of (111) 7×7 is exactly coincident with 14 unit cells of bulk-terminated (112), there is no corresponding coincident combination on the (335) surface. Given a single 7×7 unit cell as one side of the sawtooth and (337) as the opposing side, the resulting nanofacet must consist of $2\frac{1}{3}$ units of (337) and $4\frac{2}{3}$ units of (335). A coincident structure utilizing both an integral unit cell base of (335) and a single (111) 7×7 unit cell can be achieved, however, if a base of five units of (335) is combined with two of (337) and a single unit cell of (112) at the top of the sawtooth (dashed lines). This combination is consistent with the observed structure of the nanofacets on this surface, where one to three units of (337) are typically capped by a ~10 Å wide disordered region. [The disordered area presumably corresponds to the (112) unit.]

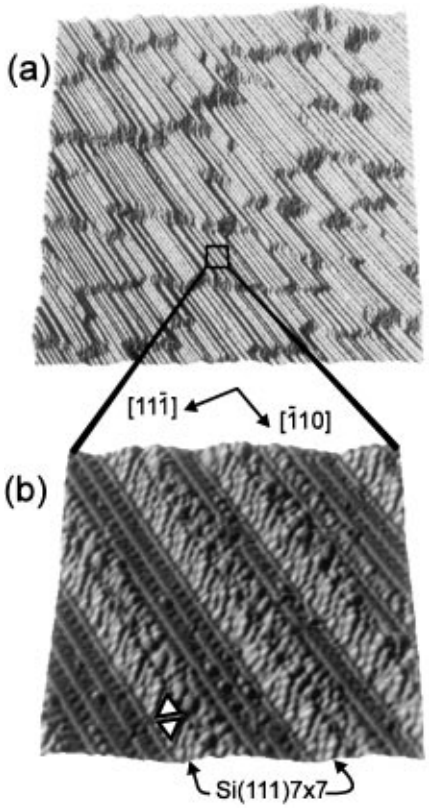

FIG. 4. Images of Si(335) revealing a nanofacet structure very similar to Si(112). (a) 5000 Å × 5000 Å image (46 Å height range). The step bunches running approximately along [111] arise from a slight miscut of the wafer. (b) 300 Å × 300 Å image (12 Å height range) showing the (337) and (111) nanofacets. One 7×7 unit cell is highlighted.

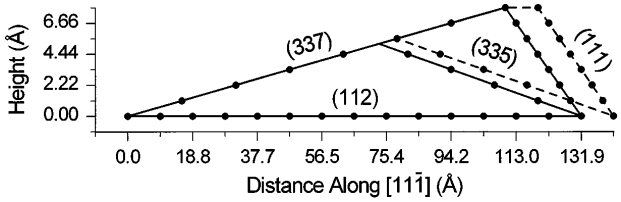

FIG. 5. Illustration of nanofacets on Si(112) and Si(335) which are composed of only a (337) terrace and a (111) terrace one 7×7 unit cell wide (solid lines). Unit cell increments for the bulk-terminated surfaces are indicated by the filled circles. On the (335) surface the ideal facet structure is not coincident with the crystal structure. The dashed lines indicate a likely configuration for a coincident nanofacet on Si(335), composed of a (111) terrace one 7×7 unit cell wide, two unit cells of (337), and a single unit of (112) on top of the sawtooth.

The formation of the (337) plane is a dramatic departure from the structures observed on less vicinal surfaces, indicating that on the more vicinal substrates studied here the free energy of a reconstructed (337) surface must be lower than that associated with multilayer-height steps. Our recent studies of atomic hydrogen adsorption on Si(112) demonstrate that the (337) facets are extremely inert [about an order of magnitude more inert than Si(100) 2×1] [14], indicating that there is a very low density of dangling bonds on reconstructed Si(337). This suggests that reconstructed Si(337) is a low energy surface, which would account for the formation of nanofacets with (337) and (111) 7×7 faces on highly vicinal surfaces. In fact, there has been previous evidence for the stability of Si(337) in studies of faceting on curved Si crystals [18,19].

In conclusion, we find that the Si(112) surface is composed of quasiperiodic, nanometer-scale facets of reconstructed (337) and (111) terraces. Similar nanofaceting is also observed on Si(335), suggesting that it is a general phenomenon for Si surfaces tilted away from (111) towards [$\bar{1}\bar{1}2$] from $\leq 14.4°$ to $\geq 19.5°$. These unique nanofacets result from the low free energy of a single unit cell of the Si(111) 7×7 reconstruction combined with the apparent stability of reconstructed Si(337). The dimensions of the nanofacets should make Si(112) and Si(335) interesting substrates for the growth of corrugated superlattices. In addition, the apparent stability of Si(337) suggests that it may make a good substrate for heteroepitaxy and quantum wire growth. Both experiments and calculations aimed at determining the structure and possible applications of Si(337) are underway.

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[15] It is important to note that Si(112) surfaces without pinning sites are completely nanofaceted (type-I regions only). However, in the absence of pinning sites, step bunches associated with the slight miscut of the wafer significantly disrupt the periodicity of the nanofacets. In contrast, when pinning sites are present the step bunches aggregate at these sites, leaving the remaining surface (type I) clean and step free. Therefore, we present an image of Si(112) with pinning sites [Fig. 2(a)] to best illustrate the quasiperiodic nanofacet structures expected for a perfectly oriented surface. Furthermore, the type-II regions caused by the pinning sites are relevant to this Letter because they resemble structures shown in a previous STM study of Si(112) (Ref. [9]).
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